Regional Scale Assessments and the Atmospheric Fate and Transport of Air Toxics: CMAQ

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July 16, 2003

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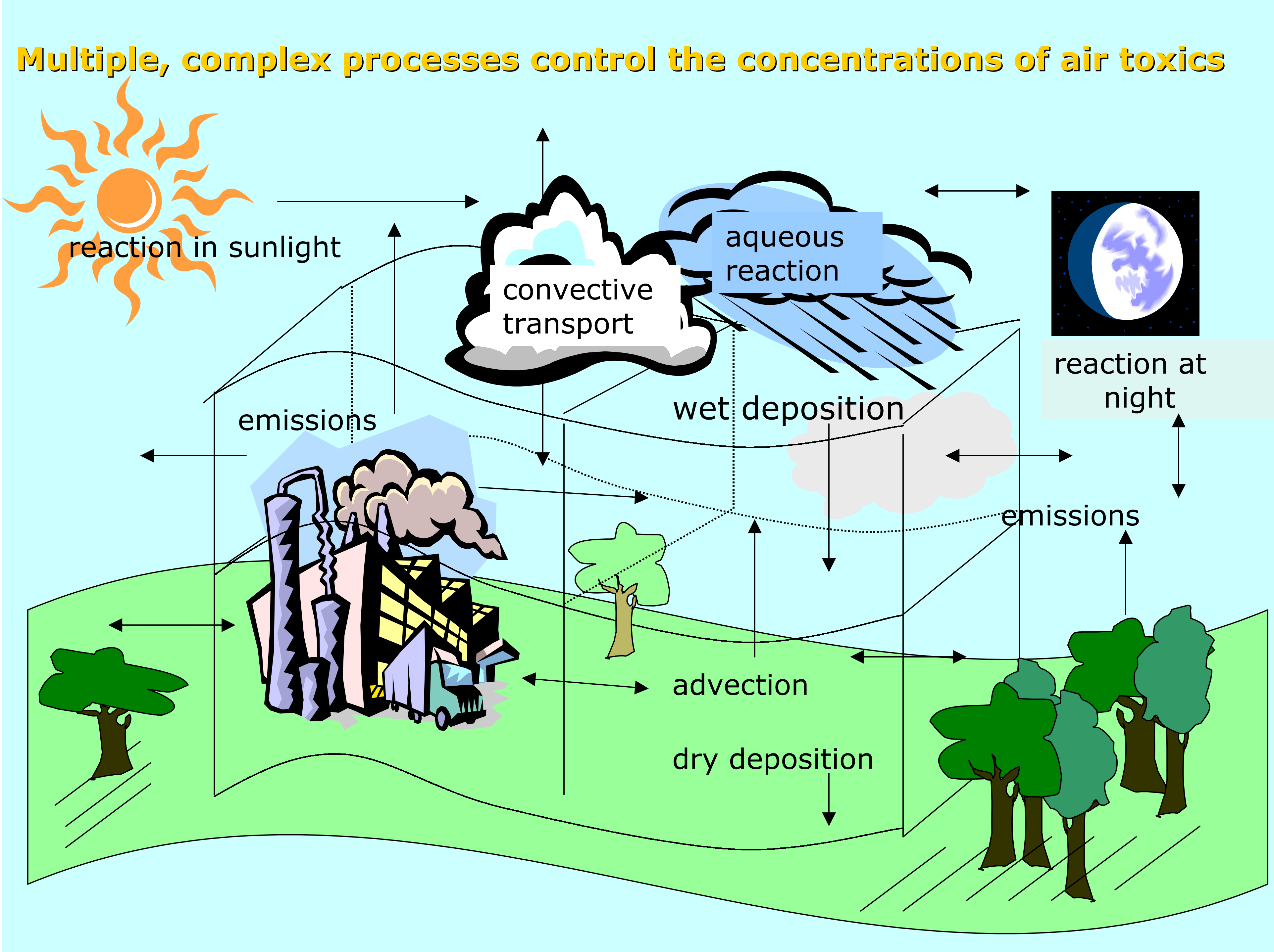
Outline

- Why it is difficult to determine atmospheric concentrations of air toxics
- How we are solving these problems using an Air Quality Model (CMAQ)
- Where and when using this approach makes a difference
- What we are planning to do in future – how this can be used by States and Regional offices


Multiple, complex processes control the concentrations of air toxics
reaction in sunlight
convective transport
aqueous reaction
reaction at night
wet deposition
emissions
emissions
advection
dry deposition

Air toxics in the atmosphere…

- Exist as gases, particles, both gases and particles, or in aqueous phase
- Have half-lives varying from a few minutes to over 2 years
- Can be produced in the atmosphere from other HAPs and non-HAPs
- Are temporally variable – they have large diurnal variations
- Are spatially variable – both vertically and horizontally

Why currently-used methods don’t address this complexity

- Monitoring
  - Can’t get the spatial distribution
  - Not always available at all times and places
- Dispersion modeling
  - Doesn’t account for wind shear
  - Can’t track plumes beyond 50 km
  - Can’t handle chemistry correctly
  - Doesn’t include biogenic sources

A more accurate way is to use an Air Quality Model, such as CMAQ

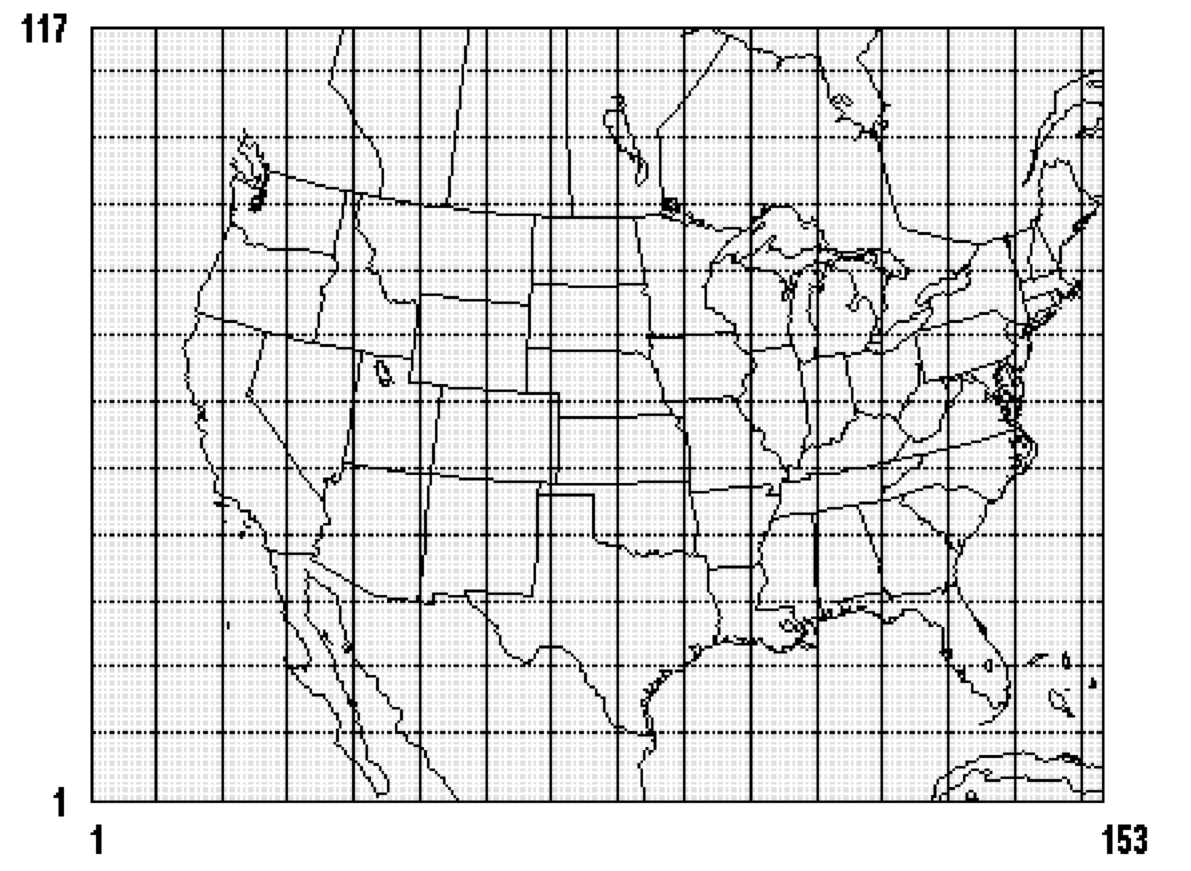
- ➔Eulerian-based (gridded) modeling system
- ➔Simulates urban and regional-scale transport and chemical processes
- ➔Gives hourly predictions with a user-defined horizontal grid resolution
- ➔Previous applications to ozone, acid rain and PM
- ➔Adapted to simulate the atmospheric fate of air toxics

First application is for the National Air Toxics Assessment (NATA)

- 36 km horizontal grids, 15 vertical layers
- hourly concentrations over a full year
- Full year of meteorological files, including 3-D wind fields, temperature, pressure, humidity, etc.
- Emissions based on merged inventories of criteria and toxics emissions

NATA Model domain

36-km grids across the continental U.S.



272,580 grids

First application is for the NATA (cont.)

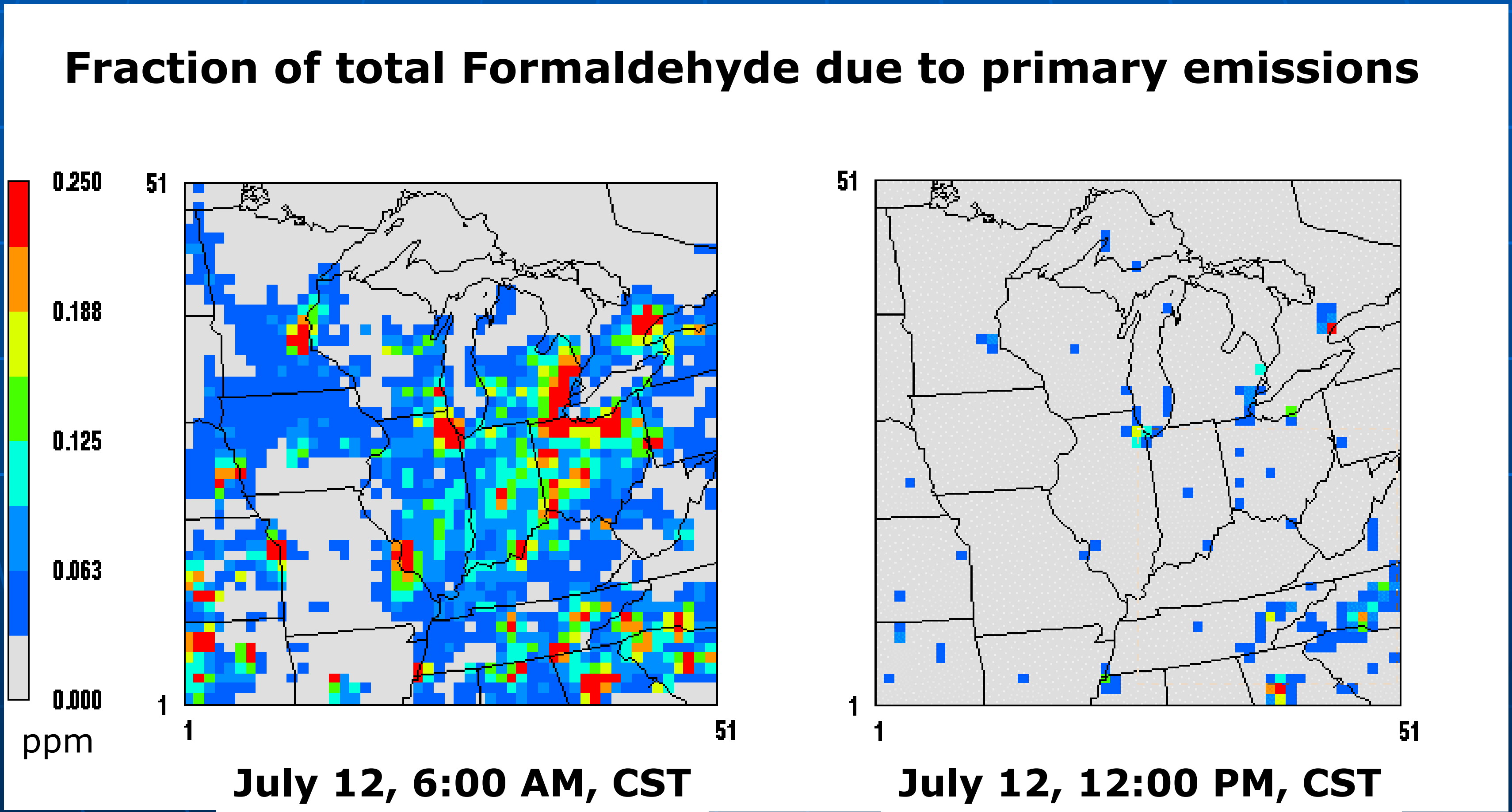
- Will include a wide range of gas phase air toxics, including those that are produced from non-toxic VOC emissions
- Includes chemical reactions from photolysis, reaction with OH, NO3, O3, and other species as appropriate
- Separates out primary (emissions) from secondary production

acetaldehyde	carbon tetrachloride	ethylene oxide	propylene dichloride
acrolein	chloroform	formaldehyde	Quinoline
acrylonitrile	1,3-dichloropropene	methylene chloride	tetrachloroethane
1,3-butadiene	ethylene dibromide	napthalene	trichloroethylene
benzene	ethylene dichloride	perchloroethylene	vinyl chloride

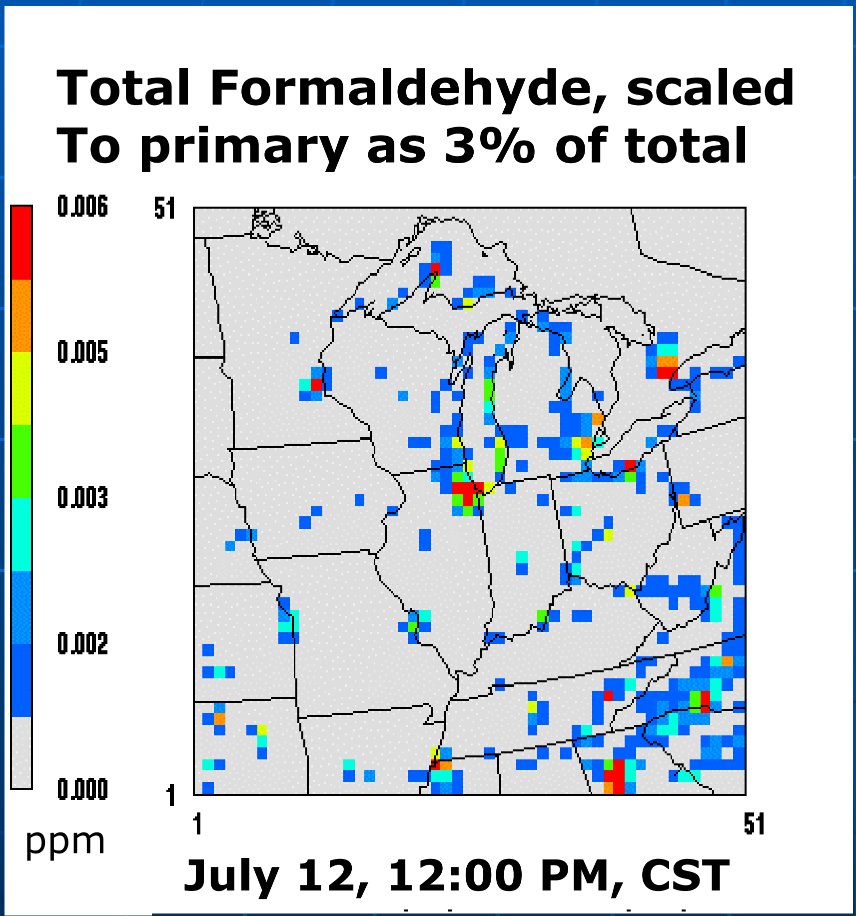
When does the use of CMAQ make a difference?

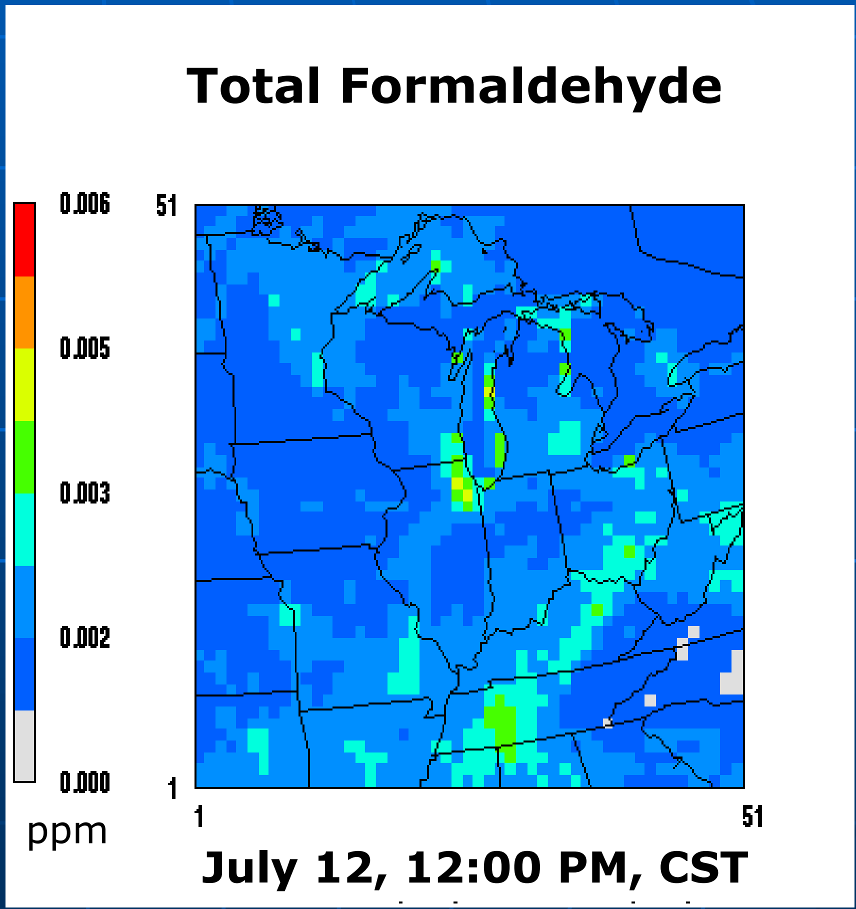
- When you need to model species, such as formaldehyde and acetaldehyde, for which secondary production is more important than their direct emissions

Secondary Production from other VOCs is the dominant source of atmospheric formaldehyde

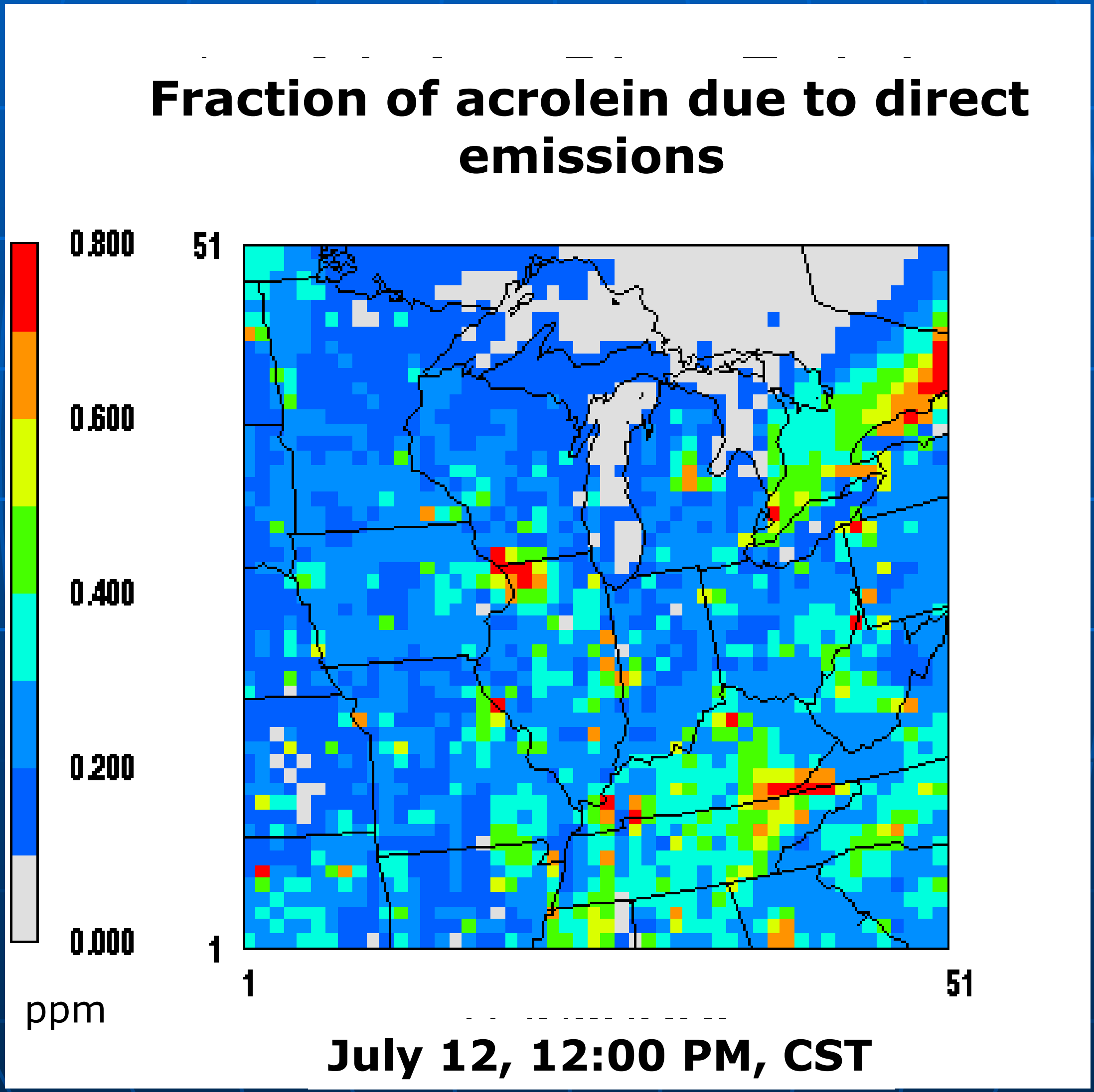


There is no easy "fix" to account for secondary formaldehyde





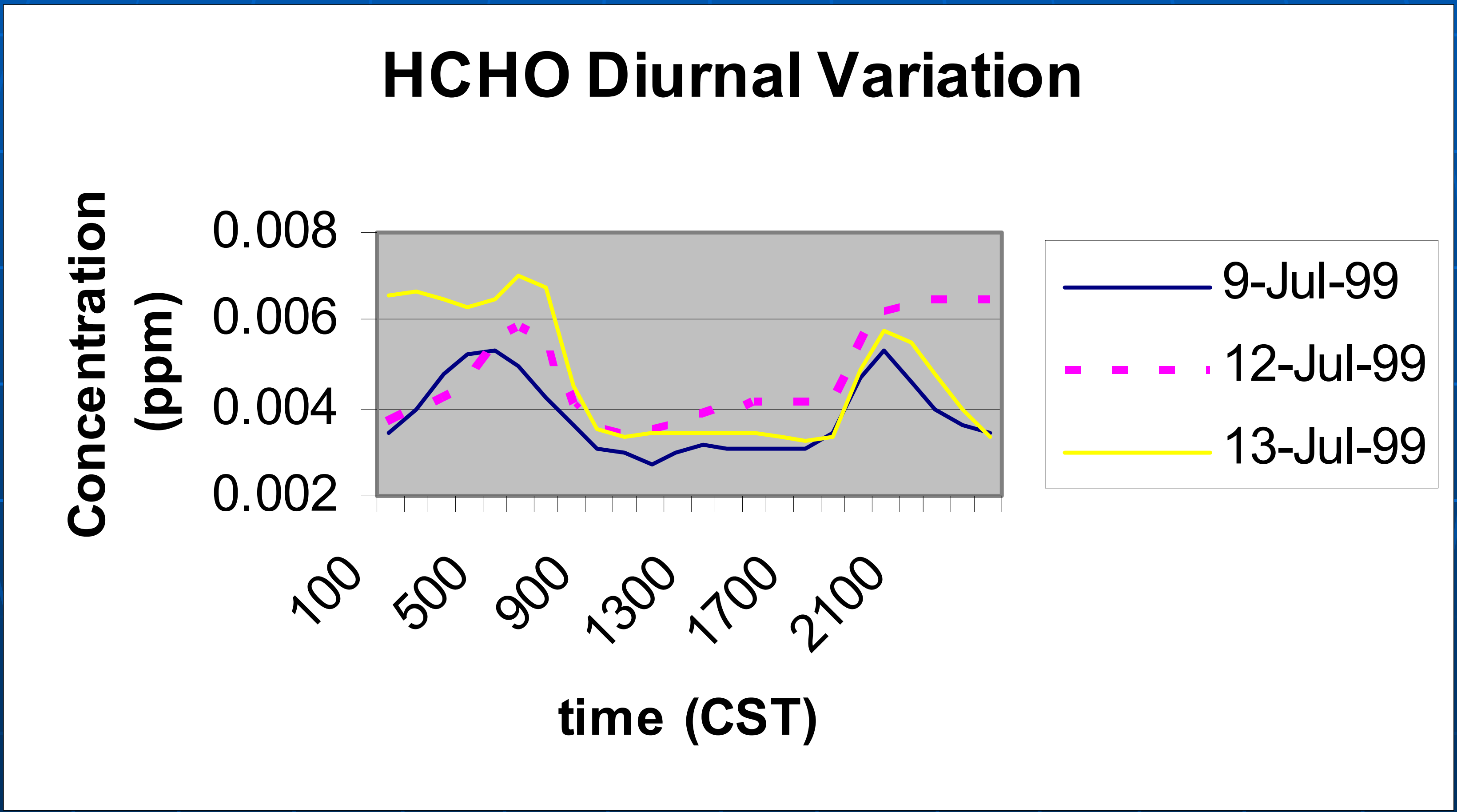
Other chemicals can also have significant, but variable secondary production



When does the use of CMAQ make a difference?

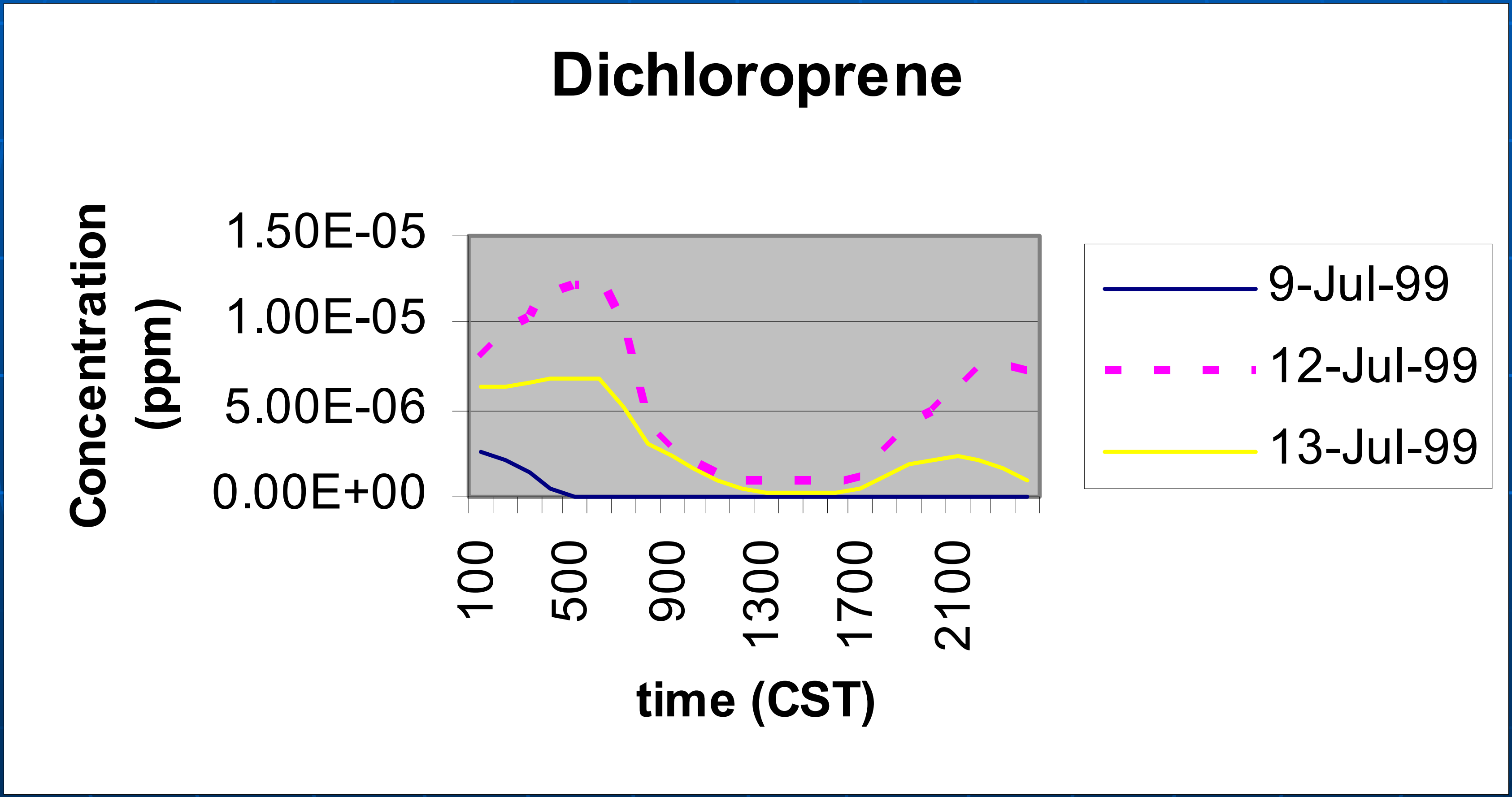
- When you need to model species, such as formaldehyde and acetaldehyde, for which secondary production is more important than their direct emissions
- When hourly and daily variations in concentrations are significant

HCHO is diurnally variable – and each day is slightly different



HCHO concentrations at grid (26,27) over Chicago

Many other air toxics also have a distinct, diurnal profile that varies from day to day



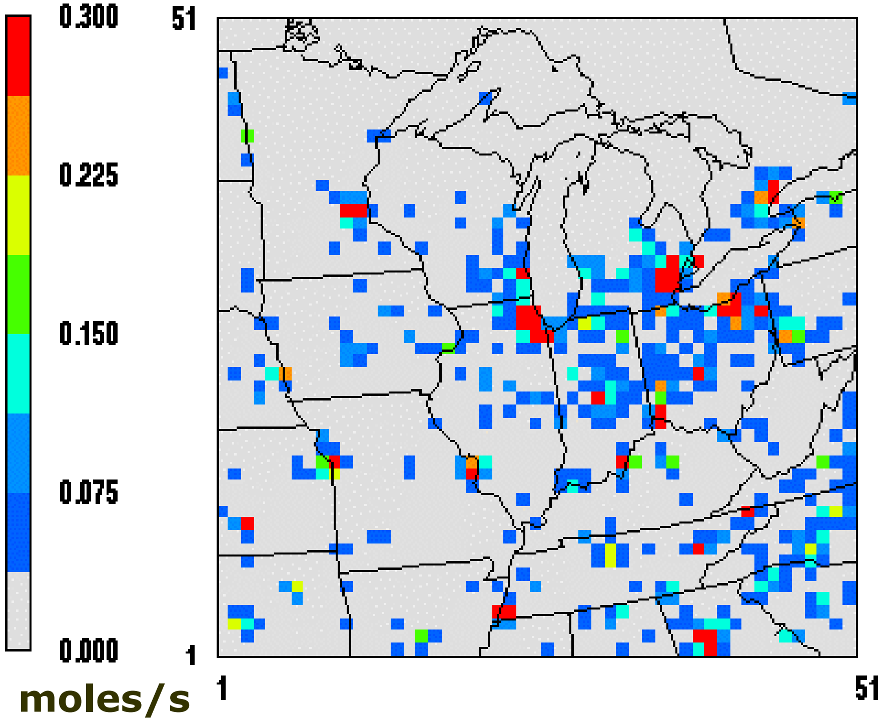
Dichloropropene concentrations at grid (38,32) in eastern Michigan

When does the use of CMAQ make a difference?

- ➔When you need to model species, such as formaldehyde and acetaldehyde, for which secondary production is more important than their direct emissions
- ➔When hourly and daily variations in concentrations are important
- ➔For compounds that are transported long distances

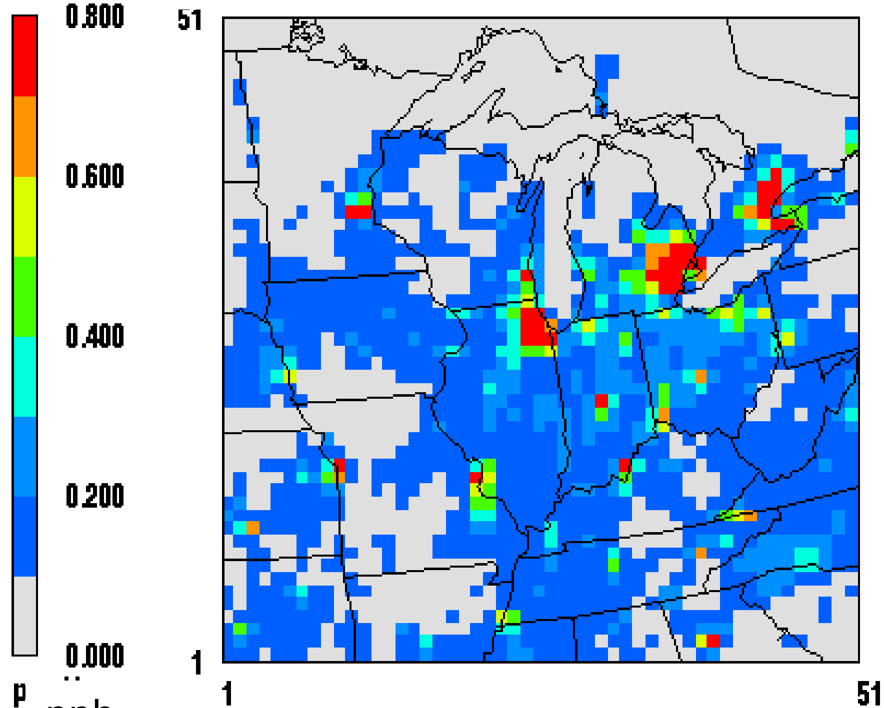
Some air toxics can be transported many miles from their sources

Benzene Emissions



July 12, 6:00 AM, CST

Benzene Concentrations



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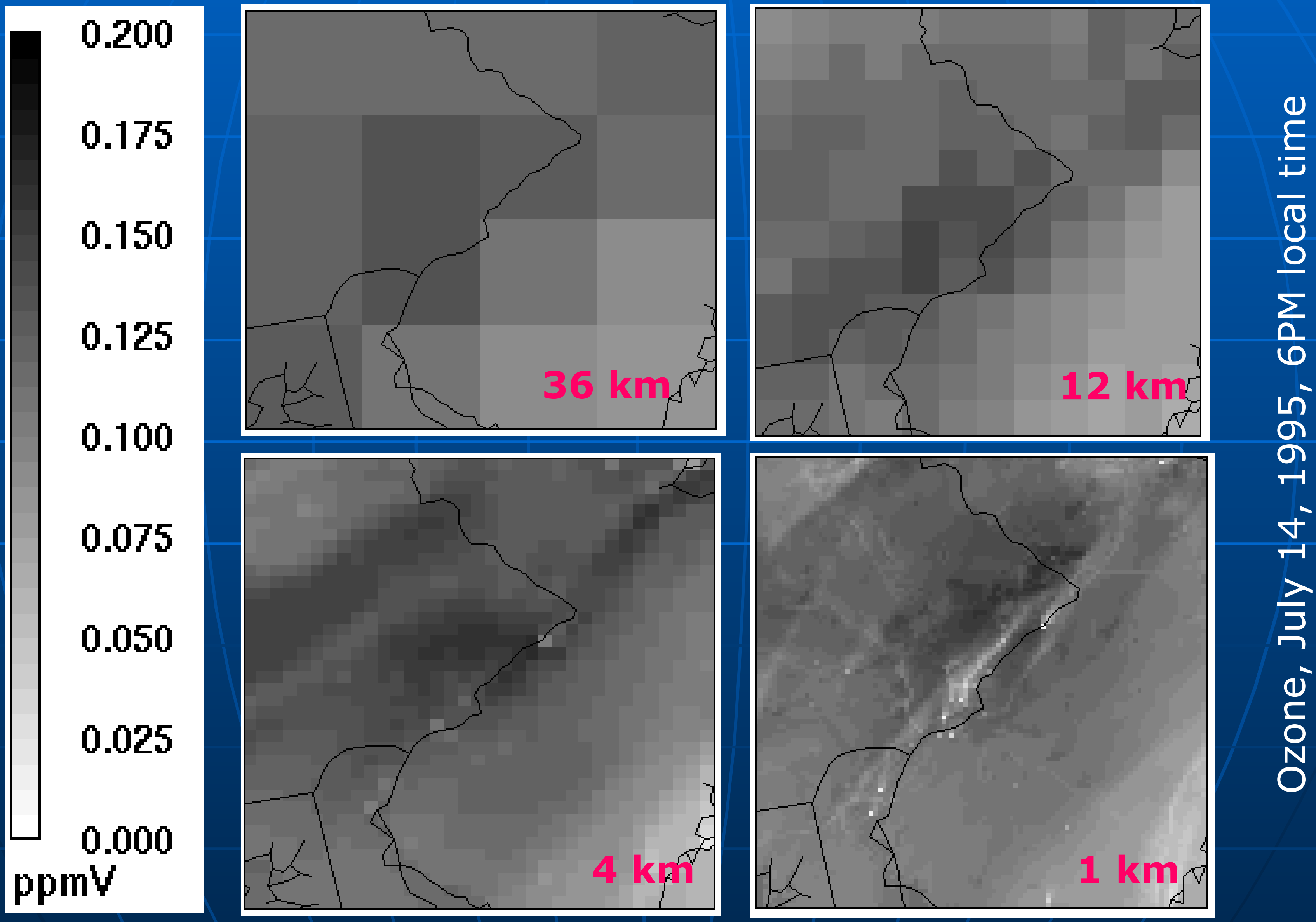
Disadvantages/Advantages of Air Quality Models

- Input data needs are intensive – including emissions, meteorology, initial and boundary conditions
  - **But better representation of important processes will provide better input for risk assesments**
- Computational processing takes a long time, depending on size and resolution of the domain
  - **But inexpensive computational resources are becoming available**
- Input and output files are large
  - **But will provide more detailed output information for risk modeling**
- Can’t get “hot spots” for less than 1 km
  - **We’re working on that**

What are we planning to do in the future?

- Simulations will nest down to 2 km, using the results from the continental simulation
- The list of toxics simulated will be expanded to include species such as metals, particle-bound toxics
- "Hot spot" concentrations will be introduced via interfacing with fine-scale techniques

More structure is apparent when “nesting” down from regional to fine scale



Summary

➔ An air quality model is essential to:

- predict the atmospheric concentrations of secondarily-produced toxics such as formaldehyde, acetaldehyde, and acrolein,
- capture the diurnal and daily variations in reactive toxics concentrations, and
- asses the long-range transport of air toxics far from their sources

Summary (cont.)

- The CMAQ model is being applied for air toxics applications
  - First output will be continental US simulation
  - First simulations are for high priority gas-phase toxics
  - Follow-up simulations will nest down over several urban areas and/or include additional toxic compounds
  - Prioritization depends on input from Program Offices, States, etc.
- For more information about CMAQ, go to http://www.epa.gov/asmdnerl/models3/CMAQ/index.html